

Tetraethylenepentamine
112-57-2 | DTXSID7026108

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.87 | 0.81 | 0.87 | 0.82 | 0.86 | 0.86 |

Model Results

Predicted value: 13.1 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.35e-01

Confidence level: 3.72e-01

Nearest Neighbors from the Training Set

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Tetraethylenepentamine

Measured: 34.5

Predicted: 13.1

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Triethylenetetramine

Measured: 32.6

Predicted: 21.3

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N,N,N',N'-

Tetramethylsuccinamide

Measured: 3.19

Predicted: 2.64

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Cantharidin

Measured: 1.53e-04

Predicted: 1.23e-03